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Volume 28

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Interdisciplinary Applied Mathematics

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Robert E. Wyatt

Quantum Dynamics with Trajectories

Introduction to Quantum Hydrodynamics

With Contributions by Corey J. Trahan

With 139 Figures

Springer

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Preface

Remarkable progress has recently been made in the development and application of quantum trajectories as a computational tool for solving the time-dependent Schrödinger equation. Analogous methods for stationary bound states are also being developed. Each year, there have been significant extensions and improvements in the basic methodology, and applications are being made to systems with increasing complexity and dimensionality. In addition, novel quantum trajectory methods are being developed for a broad range of dynamical problems, such as mixed quantum–classical dynamics, density matrix evolution in dissipative systems, and electronic nonadiabatic dynamics.

The purpose of this book is to present recent developments and applications of quantum trajectory methods in the broader context of the hydrodynamical formulation of quantum dynamics. Although the foundations of this field were established during the first 25 years following the birth of quantum mechanics, the emphasis until recently was on interpretation rather than prediction. David Bohm's 1952 publications were especially important in establishing the foundations of this field. Methodological developments occurring during and after 1999 have made it possible to use quantum trajectories to evolve wave packets for nonstationary quantum states. The equations of motion for these trajectories are readily derived from the time-dependent Schrödinger equation and are obtained without approximation. These trajectories evolve under the influence of both classical and quantum forces, the latter bringing in all quantum effects.

Although about six chapters of this book deal with Lagrangian quantum trajectories, in which the velocity matches that of the probability fluid, other chapters deal with what will be termed post-Lagrangian quantum trajectories. In the taxonomy of quantum trajectories, Lagrangian ("Bohm-type") trajectories share part of the spectrum with non-Lagrangian trajectories, the latter following extended equations of motion with additional dynamical terms that take into account "slippage" between the probability fluid and the moving grid point. In this book, these non-Lagrangian trajectories are introduced in the broader context of adaptive moving grids, which also play a significant role in classical fluid dynamics. An important advantage of these trajectories is that they eliminate some of the problems that can arise when Lagrangian trajectories are propagated. Other extensions beyond

traditional Lagrangian quantum trajectories have to do with stationary states. For these states, "pure" Lagrangian trajectories have what some view as a rather bizarre feature: they do not move at all. Extensions of the formalism to allow for quantum trajectories for which there is nonzero flux are described in the last two chapters.

There are many state-of-the-art topics covered in the following chapters that are unique to this book, including the following (not a complete list):

- The quantum trajectory equations are derived from both the Madelung–Bohmian position space and the Takabayasi phase space viewpoints.
- Detailed discussion is presented on the properties of quantum trajectories near wave function nodes.
- Evidence for Lagrangian chaos in quantum trajectory dynamics is explored, and the connection with quantum vortices is indicated.
- Function and derivative approximation on unstructured moving grids, such as those formed by Lagrangian quantum trajectories, is treated in detail.
- Adaptive moving grids for non-Lagrangian quantum trajectories are developed and applied to several examples.
- Adaptive methods for smoothing over singularities and for linking solution methods in different spatial domains are described.
- Applications to barrier scattering, decay of metastable states, and electronic energy transfer are described.
- Using fits to the density or the log derivative of the density, several methods of approximating the quantum force are described and illustrated.
- Methods are described that allow for one-at-a-time propagation of individual quantum trajectories.
- Quantum trajectory evolution in phase space is described in detail, and a novel trajectory approach for propagation of the density matrix is illustrated.
- Several new approaches to mixed quantum–classical dynamics are described, and each method is illustrated with examples.
- The quantum Navier–Stokes equation is derived, and trajectory computations of the stress tensor are illustrated.
- Methods are described for dealing with problems that can arise when propagating quantum trajectories (the derivative evaluation and node problems).
- Three trajectory approaches to stationary states are described, one of which makes close contact with semiclassical dynamics.

On the pedagogical side, a number of sections in the first half of this book (especially in Chapters 2 and 4) will be accessible to students who have had at least one course in quantum mechanics. (The reading guide in Section 1.15 lists the sections recommended for beginning students.) Some of the early chapters have been used in my graduate quantum mechanics course, and these concepts have also been presented in an undergraduate course in quantum mechanics. A simplifying aspect is that all of the trajectory equations of motion can be derived from the time-dependent Schrödinger equation by using just one elementary mathematical operation, that being differentiation. Students in elementary quantum courses who do not fear differentiation can work through the basic equations in Chapter 2

in about an hour! Also, for those wanting to go further and try it themselves, a quantum trajectory computer program is listed in Appendix 2. To provide context for the more recent developments, 11 historical comments are dispersed through the chapters.

In addition to a thorough discussion of these basic trajectory equations, there is considerable material for more advanced researchers that deals with adaptive moving grids, phase space dynamics and density matrix evolution for dissipative systems, mixed quantum–classical dynamics, and quantum trajectories for stationary states. In addition, there are about 375 references to research publications, one-third of which have appeared in the literature after 1999, and some of these results are included among the 130 figures. In order to provide background material on some topics or to give subsidiary information on specialized topics, 36 boxes containing additional information are included.

The fifteen chapters in this book cover both methodology and applications. Chapter 1 is an overview of everything that follows. It is suggested that the reader first head to Sections 1.1–1.3 for an introduction to quantum trajectories. Sections 1.4–1.13 can then be skimmed. A guide for alternative paths through the chapters is presented in figure 1.2. Chapters 2–4 cover the equations of motion and properties of quantum trajectories, and Chapters 6–9 present applications to model problems. Chapters 3 and 11 deal with phase space dynamics, but Chapter 10 should be read before Sections 11.6–11.8. Quantum trajectories for nonstationary states form the focus for Chapters 2–13, but stationary states are dealt with in Chapters 14 and 15. Problems that can arise in propagating quantum trajectories are described in Chapters 4–6, and resolutions for these problems are described in Chapters 7 and 15.

Some of the material covered in Chapters 2 and 4 overlaps material that is covered in Peter Holland's outstanding 1993 book, *Quantum Theory of Motion*. There is considerable material in Holland's book (such as spin and relativity) that is not covered in this book. However, there is a computational flavor in the present book that is lacking in Holland's book, and there are discussions here of many recent developments that, of course, could not be covered in Holland's book. In some respects, these two books complement one another.

Acknowledgments. I am very grateful for the assistance and encouragement provided by many individuals during the preparation of this book. Special thanks to Corey Trahan for writing outstanding draft versions of Chapters 6 and 7 and for revising an awkward version of Chapter 5. For a draft version of Sections 9.1–9.4, I thank Eric Bittner and Jeremy Maddox. I thank Bill Poirier for many insightful comments about the material in several of the chapters (especially Chapter 14) and for providing notes and preprints that led to some of the material in Sections 15.2 and 15.3. I thank Irene Burghardt for numerous comments that led to improved versions of Chapters 3 and 11. Edward Floyd contributed a number of comments on Chapter 14, for which I am grateful. For comments on the book, thanks to Keith Hughes and Dmytro Babyuk. For stimulating and productive collaborations

over the past five years that led to several joint publications, I am indebted to Eric Bittner. In addition, for many enlightening discussions over the past five years about the material that has ended up in these chapters, I thank Gerard Parlant, Irene Burghardt, Brian Kendrick, Sonya Garashchuk, Klaus Moller, Don Kouri, and David Hoffman. For many insightful discussions and for the numerous original contributions to quantum hydrodynamics that my students and postdoctoral scientists have made since 1998, I give special thanks to Courtney Lopreore, Corey Trahan, Keith Hughes, Dmytro Babyuk, Fernando Sales Mayor, Lucas Pettey, Denise Pauler, and Brad Rowland.

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Cover Illustration. The color illustration on the cover was designed by the visualization experts at the Texas Advanced Computing Center. Reuben Reyes, David Guzman, and Karla Vega are thanked for producing this figure (using the POV-Ray ray tracing suite) and for animating the trajectory results. These quantum trajectories, shown as colored spheres at one time step, are evolving in a four-dimensional phase space, but two spatial coordinates and one momentum coordinate were used for plotting purposes. The trajectory equations of motion for this dissipative quantum system were derived from the modified Caldeira–Leggett equation, which is described in Chapter 11. The trajectories on the right side of the figure are escaping over a barrier, while those near the center are temporarily trapped in a metastable state. The value of the phase space distribution function is largest for the interior spheres and is much smaller for the boundary ones.

Austin, Texas, USA *Robert E. Wyatt*

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Lagrange	jeff560.tripod.com/lagrange.jpg (photograph used after contacting Jeff Miller, email: Jeff560@aol.com)
Madelung	www.th.physik.uni-frankfurt.de/∼jr/gif/phys/madelung.jpg (webpage maintained by Joachim Reinhardt, email: jr@th.physik.uni-frankfurt.de)

Chapter 4

Jacobi	www-gap.dcs.st-and.ac.uk/∼history/PictDisplay/Jacobi.html (photograph used after contacting John O'Connor, email: joc@st-andrews.ac.uk)

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1
Introduction to Quantum Trajectories

Quantum trajectories provide an analytical, interpretative, and computational framework for solving quantum dynamical problems. An overview is presented of methods and applications for both nonstationary and stationary quantum states.

1.1 Dynamics with Quantum Trajectories

The Schrödinger equation for both stationary and nonstationary states may be solved exactly by propagating *quantum trajectories*, at least *in principle*. The probability amplitude and the phase of the wave function are transported along these trajectories and observables may be computed directly in terms of this information. The dynamical theory governing quantum trajectories forms part of the *hydrodynamic formulation of quantum mechanics*, the logical foundations of which were established by de Broglie, Madelung, Bohm, Takabayasi, and others. Distinct from, but related to the hydrodynamic formulation is the *de Broglie–Bohm interpretation of quantum mechanics*. The foundations for these approaches were developed during the period 1926–1954, although almost nothing happened for 25 years between 1927 and 1952 [2.2, 2.3, 2.9, 3.1]. However, after another long gap, new methods for computing quantum trajectories were introduced in 1999, and this helped to create a resurgence of interest in the hydrodynamic formulation. Since then, more robust computational methods have been developed, and quantum trajectories are now being applied to a diverse range of problems, including some that were probably not anticipated by the early workers, including phase space dynamics for open quantum systems, mixed quantum–classical dynamics, and electronic nonadiabatic energy transfer.

Depending on how they are computed, investigations that employ quantum trajectories may be broadly divided into two classes. In the older and quite mature de Broglie–Bohm *analytic approach*, the time-dependent Schrödinger equation (TDSE) is first solved using conventional computational techniques (using space-fixed grids or basis set expansions). Then, individual "particles" or corpuscles are

evolved along quantum trajectories $\vec{r}(t)$ with velocities generated by the "ψ-field", $d\vec{r}/dt = (\hbar/m)\,\mathrm{Im}[\vec{\nabla}\ln\psi]$. The patterns developed by these quantum trajectories as they emanate from an ensemble of "launch points" exactly define the history of the system as it evolves from the initial to the final state. The value of the synthetic route is "a means of understanding and exploring quantum behavior, that is, as a heuristic tool" [1.16]. This is the approach that was proposed and developed by de Broglie, Bohm, and others, the purpose of which is *not* to solve the TDSE per se, but to provide insight. Frequently, interpretative terms such as "pilot wave", "ontological status of the wave function", and "hidden variables" are associated with this approach. A survey of the de Broglie-Bohm interpretation is presented by Berndl et al. [1.23], and Tumulka [1.24] has presented a "dialogue" which explores many aspects of this approach. Finally, Dürr's book [1.25] *Bohmsche Mechanik als Grundlage der Quantenmechanik* provides a detailed exposition. Dürr et al. have also extended Bohmian mechanics to quantum field theory [1.34].

Since the time that Bohm's two papers were published, the analytic approach has been used to compute and interpret quantum trajectories for a diverse spectrum of physical processes, including diffraction experiments, barrier and dynamical tunneling, beam scattering from solid surfaces, and currents in molecules and electronic devices. As an example of the synthetic method, Sanz et al. studied the final angular distribution of quantum trajectories for the scattering of He atoms from corrugated Cu(110) surfaces [1.15]. In another example, Wang et al. used quantum trajectories to study the dissociative adsorption of $D_2(v = 0,1,2)$ on Cu(111) surfaces [1.14]. A detailed force analysis was carried out for the unique group of trajectories that make it into the dissociation channel. A third example concerns the analysis by Barker et al. of current distributions in quantum dots [1.22]. Many insights have been gleaned from these and related studies, some of which will be described in the following chapters (see especially Sections 4.10 and 4.11, 13.5–13.7, and 13.8 which deal with chaotic trajectories, vortex dynamics, and dynamical tunneling, respectively).

The second category of quantum trajectory methods follows the *synthetic approach*. Rather than guiding quantum trajectories with a precomputed wave function, *the trajectories and the hydrodynamic fields are computed concurrently, on the fly*. In this approach, wave packets are evolved by propagating ensembles of quantum trajectories, which become the *computational tool* for solving the quantum hydrodynamic equations of motion (QHEM). Rather than being fixed in space as in the Eulerian picture of fluid mechanics, these fluid elements move along with the probability fluid. In the special case that these elements move at the flow velocity of the fluid, this is termed the Lagrangian version of the formalism. The total force guiding each quantum trajectory includes the classical force (from the gradient of the "external" potential) plus the quantum force (from the gradient of the *quantum potential*). The latter depends on the *shape of the density surrounding each trajectory* and brings in all quantum effects. (As mentioned previously, Bohm's work was not especially concerned with this approach; rather, the focus was on "corpuscle propagation" using information gleaned from precomputed wave functions.)

The hydrodynamic formulation in the synthetic approach is considerably more than "just an interpretation"; it presents nontraditional computational techniques for solving quantum dynamical problems in addition to utilizing the descriptive terminology of fluid mechanics. An insightful analysis of trajectory approaches to quantum mechanics and their relationship to "wave pictures" has been presented by Holland [1.33].

The first implementation of the synthetic approach, the *particle method*, was developed by Weiner et al. during the period from the late 1960s through the 1970s. The computational techniques used in these studies were effectively limited to Gaussian wave packets evolving on harmonic potential surfaces [4.17, 4.18]. (Surprisingly, the first few of these papers made no mention of the much earlier work by Bohm.) Stimulated by these studies, a number of workers (including the author of this book!) attempted to use the same computational methods for wave packet evolution on anharmonic potentials, but the algorithms were too immature to permit even short time propagation. Following these early successes and failures, there was another long gap. Then, in 1999, two groups, working independently, published studies in which ensembles of quantum trajectories were evolved on anharmonic potentials. The first of these, by Lopreore and Wyatt [4.1], introduced a computational approach called the *quantum trajectory method*, QTM. The other study, by Sales Mayor, Askar, and Rabitz [4.2], developed what was called *quantum fluid dynamics*, QFD. Although different computational methods were employed, both methods solve the QHEM by evolving ensembles of quantum trajectories. (The main difference between the first QTM and QFD papers was the method used to evaluate spatial derivatives of the density and the velocity, quantities that are needed in the QHEM.)

We have already hinted that the QHEM can be solved in a number of different *pictures* (there are actually an infinite number of possibilities). In the *Eulerian picture*, fluid elements (grid points) are stationary, while in the previously mentioned *Lagrangian picture*, grid points move along trajectories with velocities matching the flow velocity of the probability fluid. In many cases, alternative pictures (referred to as the ALE, or *arbitrary Lagrangian–Eulerian picture*) that allow for *adaptive grid point motion* are more useful than the standard Eulerian or Lagrangian pictures. (Just to set the record straight, the Eulerian and Lagrangian pictures were both introduced by Euler, but it would be confusing to refer to them as "Euler I" and Euler II".) The Lagrangian and ALE pictures, in which trajectories are used to solve QHEM, provide a very different computational approach from those used in conventional formulations quantum dynamics. Perhaps it is worth emphasizing that the QHEM *can be* solved in the Eulerian picture, for example, by discretizing the equations of motion on a rigid space-time lattice. However, the full power and elegance of the hydrodynamic formulation are exposed only by *evolving quantum trajectories* in the dynamical pictures mentioned previously.

Why solve the hydrodynamic equations with *quantum* trajectories? A number of reasons are summarized in Box 1.1, but an appealing feature is that the *exact* quantum mechanical equations are being solved. *The predictive power of the*

Box 1.1. Why run quantum trajectories in the synthetic approach?

1. Exact quantum-dynamical equations of motion are solved.
2. The trajectories follow the evolving probability density.
3. A relatively small number of moving grid points (fluid elements) may be needed.
4. $x(t)$ describes where the "particle" has been, and dx/dt tells where it is going next.
5. The equations of motion bring in elementary dynamical concepts, such as forces.
6. The trajectories can be used for informative analysis, such as phase space plots.
7. New insights may arise, because the trajectories show how the process takes place.
8. New computational approaches can be developed (e.g., for density matrix evolution for mixed states and for mixed quantum–classical dynamics).
9. The computational effort scales linearly with the number of trajectories.
10. Can possibly avoid the traditional exponential scaling of computational effort with respect to the number of degrees of freedom.
11. There are no large basis sets or large fixed grids.
12. There is no need for absorbing potentials at the edges of the grids.

synthetic approach is equivalent to that of conventional quantum mechanics. In addition, these trajectories may provide a very economical way of solving the TDSE, because the trajectories follow the main features of the evolving probability density. With further improvements in the computational methods, quantum trajectory evolution may provide a robust approach for systems with more degrees of freedom than can be handled using fixed-grid methods. Another compelling reason for running quantum trajectories is that we may *gain new insights* into the dynamics. Unlike conventional computational methods, quantum trajectories provide detailed information about *how* the process takes place. These insights may lead to improved algorithms for treating systems of increasing complexity and dimensionality. This has already started to happen, as evidenced by the number of studies being reported each year. It is hoped that the prejudice displayed by some against the use of trajectories in the analytic approach will not carry over to the synthetic approach!

The appealing features of trajectories are certainly well known to those who solve dynamical problems by running classical or semiclassical trajectories. However, it is important to distinguish formally exact quantum trajectory approaches from those that "simulate" quantum dynamics in terms of classical or semiclassical trajectories, even though the latter can provide accurate and insightful results for some problems.

Unfortunately, the propagation of quantum trajectories can be problematic. In fact, using the simplest computational implementations of the basic equations of motion, there are several numerical problems that limit the propagation time of

quantum trajectories, at least for some problems. The first of these is the *derivative evaluation problem*. In order to integrate the QHEM for quantum trajectories, spatial derivatives of the hydrodynamic fields are needed at the positions of the moving fluid elements. However, because these elements move at different velocities (even in the absence of an external potential), at each instant of time they form an unstructured grid, even if they were launched from a regular grid. The accurate computation of spatial derivatives, given only the function values at a set of scattered points, is a difficult problem in numerical analysis. Provided that the input fields are relatively smooth, there are several fitting algorithms, such as least squares, that provide reasonable approximate solutions to the derivative problem.

In addition to these fitting methods, there is another approach that is even more effective. Borrowing ideas from classical computational fluid dynamics, it is possible to *design moving grids* with a predetermined structure, including those with equally spaced internal points. The edge points are allowed to move, thus permitting overall translation as well as internal expansion or contraction as needed. Modifications must be made in the equations of motion to allow for these *non-Lagrangian paths*, thus leading to the *moving path transforms* of the original equations of motion. On these structured grids, standard algorithms (such as high-order finite difference or pseudospectral methods) can be used to accurately evaluate the spatial derivatives. This approach effectively solves the derivative evaluation problem.

Two additional problems concern trajectory dynamics in *nodal regions*. Near nodes associated with nonstationary states, the quantum potential undergoes rapid variations over short length scales and is singular at the exact nodal position. The first difficulty that arises in these regions is that the equations of motion for the quantum trajectories become *stiff*, meaning that that the solutions contain modes with vastly different scales in space and time. Fortunately, there are a number of excellent *implicit time integrators for stiff systems*. Although not optimal insofar as the time step is concerned, even the explicit Euler method will provide reasonable results. With use of the appropriate algorithms for stiff differential equations, the *stiff equation problem* is soluble.

The second problem that occurs in nodal regions is much more severe than those mentioned previously. In these regions, quantum trajectories may become difficult or even *impossible* to propagate accurately (using the simplest implementations of the integration algorithms). The trajectories become kinky and unstable, leading to bizarre dynamics and sudden death for the executing computer code. The use of adaptive grids helps significantly, but does not eliminate the problem. Much effort has been spent on developing methods to deal with *the node problem*. Fortunately, several ways have been found to circumvent this problem, including the use of smoothing potentials in nodal regions or the use of hybrid algorithms that combine solutions of the TDSE in the nodal regions with solutions to the hydrodynamic equations in other regions. There have been successful applications of these methods that lead to stable and accurate long-time propagation even when multiple nodes form. However, it turns out that there are other ways to "cope with the node problem", and three promising new methods developed for this purpose

will be described in the final chapter of this book. Two of these methods are based on the propagation of *node-free functions.*

The emphasis in this book is on computational implementations of the synthetic route to wave packet propagation using quantum trajectories. *The focus will be on the equations of motion for quantum trajectories, the computation and properties of these trajectories, and their application to physical and chemical problems.* A number of methods are described for propagating these trajectories, and many properties of quantum trajectories are illustrated through applications to model problems. Many of these applications are for one-dimensional model problems, but a few apply to problems in much higher dimensionality. The literature on applications of quantum trajectory methods to stationary quantum states is relatively sparse. However, three approaches devised for these states will be described in Chapters 14 and 15. In the following chapters, quantum trajectory approaches developed during and after 1999 will be applied to a number of processes, including barrier tunneling, electronic transitions, decoherence, and mixed quantum–classical dynamics. In addition, new quantum trajectory approaches will be described for evolving the density matrix and the phase space distribution function for dissipative quantum systems.

Regarding item number 10 in Box 1.1, it is frequently mentioned that conventional computational methods for solving the Schrödinger equation *scale exponentially* with respect to the number of degrees of freedom. As pointed out by Poirier, this is not a fundamental limitation; rather, it is an artifact associated with the use of direct product basis sets [1.18]. Recently, several promising new methods may spell an end to exponential scaling [1.19–1.21]. One of these methods, which combines wavelet basis sets with phase space truncation schemes, has extended the number of degrees of freedom that may be considered from about 6 to about 15 [1.18]. Further extensions are expected in the number of degrees of freedom that can be handled on current computers.

It is not currently known in detail how methods using ensembles of quantum trajectories scale with respect to the number of degrees of freedom. Not many multidimensional studies have been performed (however, there are some examples; see [7.19, 8.2, 8.5]). A more significant feature is that the trajectories follow along with the evolving density. Because of this, it is not necessary to cover large regions where there is little activity, just in case something happens there in the future. In addition, very few trajectories are required in regions where the hydrodynamic fields are relatively smooth. However, when the dynamics become more complex (for example, when nodes and ripples form in the density), additional trajectories are needed to resolve the details. As the dynamics develops in time, trajectories can be added or deleted, depending on the smoothness of the hydrodynamic fields. How many trajectories are required to do the job is highly dependent on the nature of the system under study and on control parameters, such as the average energy of the wave packet. As additional multidimensional examples are explored, it is expected that these scaling issues will become resolved.

The following sections of this chapter provide an overview of the main topics covered in this book, but the more technical parts can be skipped on a first reading.

An overview of two of the topics covered in this book (the use of adaptive grids and the use of fitting techniques to develop approximations to the quantum force) appeared in *Computing in Science and Engineering* [1.1].

1.2 Routes to Quantum Trajectories

As shown on the left side of figure 1.1, for nonstationary quantum states, there are two independent routes to the equations of motion for quantum trajectories. The first of these begins with the wave function expressed in position space and leads to the equations developed by Madelung and Bohm. The second route follows the work of Takabayasi and begins with the quantum distribution function expressed in phase space. We will return to the phase space approach later in this section, after the QHEM are previewed. (Although the goals are different, some of the same equations appear in both the analytic and synthetic approaches. However, there are important equations used in the synthetic approach to trajectory propagation, such as equations 1.13, 1.14, 1.18, and 1.20, which are not needed in the de Broglie–Bohm interpretation.)

There are also several routes to quantum trajectories for stationary states, all of which emphasize the importance of the quantum stationary Hamilton–Jacobi equation. The oldest of these, pioneered by Edward Floyd, leads to *Floydian trajectories*, the second one (developed by Faraggi and Matone) begins with a broad unifying concept, *the quantum equivalence principle*, and the most recent one

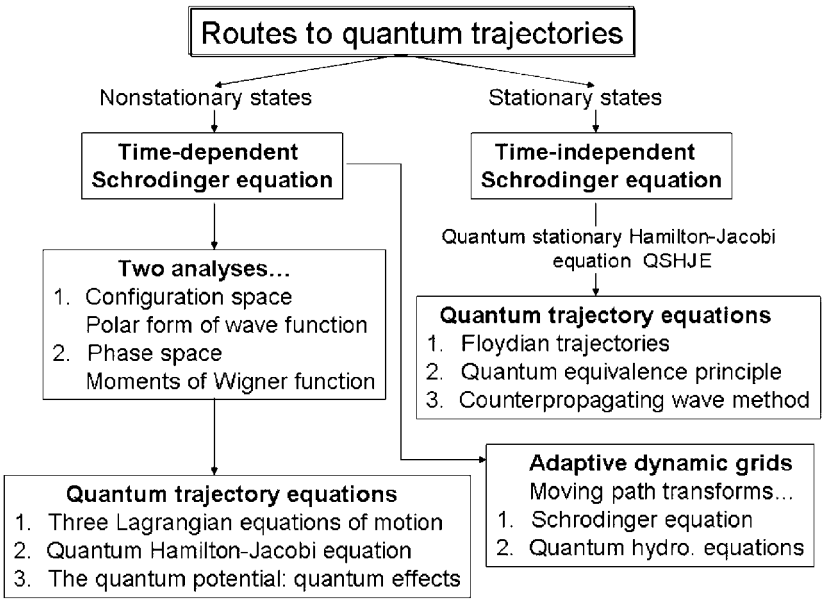

FIGURE 1.1. Routes to quantum trajectories for both stationary and nonstationary states.

(developed by Poirier) is based on expansion of the wave function in terms of *counterpropagating waves*. The latter approach provides a significant reconciliation of the hydrodynamic formulation with semiclassical mechanics. We will delay further mention of these approaches until Sections 1.12 and 1.13.

Starting from the TDSE, Madelung carried out the first derivation of the Eulerian version of the hydrodynamic equations in 1926 [2.9]. This work was greatly extended by Bohm's 1952 papers [2.2, 2.3], which showed how quantum effects, originating from the *quantum potential*, influence the motions of microscopic particles. These topics form the subject of Chapter 2, especially Section 2.2, a brief summary of which will be presented in this section.

Madelung began by writing the complex-valued time dependent wave function in polar form, given by (assuming a one-dimensional example)

$$\Psi(x,t) = R(x,t)e^{iS(x,t)/\hbar}, \tag{1.1}$$

in which both $R(x,t)$, the amplitude, and $S(x,t)$, the *action function,* are real-valued. In addition, and this is quite important, it is assumed that $R(x,t) \geq 0$ at all points. The probability density associated with this wave function is $\rho(x,t) = R(x,t)^2$. In order to develop the Eulerian version of the hydrodynamic equations, we begin by substituting equation 1.1 into the TDSE. After some manipulations, we obtain a system of two *coupled partial differential equations*. The *first equation* is the *continuity equation*

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x} = -\frac{\partial}{\partial x}\left[\rho(x,t)v(x,t)\right]. \tag{1.2}$$

The probability flux is $j(x,t) = \rho(x,t)v(x,t)$, in which $v(x,t)$, the *flow velocity* of the probability fluid, is determined by the spatial derivative of the action function,

$$v(x,t) = \frac{1}{m}\frac{\partial S(x,t)}{\partial x}. \tag{1.3}$$

The *second equation* that results from this substitution is the *quantum Hamilton–Jacobi equation*, given by

$$-\frac{\partial S(x,t)}{\partial t} = \frac{1}{2m}\left(\frac{\partial S(x,t)}{\partial x}\right)^2 + V(x) + Q(x,t). \tag{1.4}$$

Except for the final term on the right, it has the same form as the classical Hamilton-Jacobi equation for the classical action function. The first term on the right side is the *flow kinetic energy*, the second term is the "classical" potential energy, and the final term is the Bohm *quantum potential*.

Because of its explicit dependence on $\hbar$, *the quantum potential Q brings all quantum effects into the hydrodynamic formulation*. The quantum potential can be expressed in several ways, from the R-amplitude or the probability density:

$$Q(x,t) = -\frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial^2 R}{\partial x^2} = -\frac{\hbar^2}{2m}\rho^{-1/2}\frac{\partial^2 \rho^{1/2}}{\partial x^2}. \tag{1.5}$$

We note that Q depends on the curvature of the R-amplitude, as measured by the second derivative. A significant feature is the presence of R in the denominator.

Near a node in the wave function, the quantum potential becomes very large, unless it happens that the curvature of R is zero at this point. (Such inflection points occur at nodes in wave functions for bound stationary states.) In general, Q becomes very large near a node, and the sign can be either positive or negative.

It will be shown in Chapter 2 that the local kinetic energy associated with a wave packet can be decomposed into *flow kinetic energy* and *shape kinetic energy* [4.3], the latter being determined by the curvature of the amplitude. The shape kinetic energy is the same function that has been identified as the quantum potential. The quantum potential is a measure of the shape induced *internal stress*; this quantity is relieved when the packet "flattens out" as much as possible, subject to constraints imposed by the potential energy.

Prior to Bohm's work, it was appreciated that *quantum mechanics is nonlocal*: every part of a quantum system depends on every other part and is subject to organization by the whole. A significant feature of Bohm's work is that *the quantum potential was identified as the origin of nonlocality*. In addition to the classical force, the quantum potential leads to an additional force, the *quantum force*, acting to guide the trajectory. As a result, in the hydrodynamic formulation *the trajectories lose their independence* and are organized (correlated) by the quantum potential. If Q is neglected in the quantum Hamilton–Jacobi equation, then the resulting classical equations describe a *local theory*.

The preceding equations of motion for $\rho(x,t)$ and $S(x,t)$ have been expressed in the *Eulerian picture*: an observer at a *point fixed in space* watches the wave packet move by. In order to recast these equations into a form appropriate for propagating trajectories, we will take a different viewpoint. If we follow along a (yet to be determined) trajectory $x(t)$ moving with speed v, the rate of change in the function $f(x,t)$ is given by the *total time derivative*

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{dx}{dt}\frac{\partial f}{\partial x} = \frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x}, \tag{1.6}$$

in which the first term is the rate measured by the stationary observer, and the second term converts us to the moving frame. The observer following along this trajectory is in the *Lagrangian frame*, and equation 1.6 is used to convert time derivatives from the Eulerian frame into the Lagrangian frame.

We will now transform the Eulerian version of the quantum Hamilton–Jacobi equation into an equation of motion for the quantum trajectories. The first step is to transform this into an equation of motion for the spatial derivative of the action, $\partial S/\partial x$. (This procedure, developing *equations of motion for spatial derivatives*, will be significantly extended in Chapter 10.) If we operate on both sides of equation 1.4 with $\partial/\partial x$, and then use equation 1.6 to convert to the Lagrangian frame, we obtain the Newtonian-type equation of motion

$$m\frac{dv}{dt} = -\frac{\partial}{\partial x}(V+Q) = f_c + f_q. \tag{1.7}$$

The right side of this equation shows that the total force guiding the trajectory is the sum of the classical force, $f_c = -\partial V/\partial x$, and the quantum force, $f_q = -\partial Q/\partial x$.

Box 1.2. Summary of equations of motion for quantum trajectories

$$\frac{d\rho(\vec{r},t)}{dt} = -\rho(\vec{r},t)\vec{\nabla}\cdot\vec{v}(\vec{r},t), \tag{1}$$

$$m\frac{d\vec{v}}{dt} = -\vec{\nabla}(V+Q) = \vec{f}_c + \vec{f}_q, \tag{2}$$

$$\frac{dS}{dt} = \frac{1}{2m}\vec{\nabla}S\cdot\vec{\nabla}S - (V(\vec{r}) + Q(\vec{r},t)) = L, \tag{3}$$

$$Q(\vec{r},t) = -\frac{\hbar^2}{2m}\frac{1}{R(\vec{r},t)}\nabla^2 R(\vec{r},t), \tag{4}$$

$$\rho(\vec{r},t) = R(\vec{r},t)^2, \tag{5}$$

$$\vec{v}(\vec{r},t) = (1/m)\vec{\nabla}S(\vec{r},t). \tag{6}$$

This *quantum Newtonian equation*, which describes *how an object moves*, plays a major role in the hydrodynamic formulation.

The *Lagrangian version* of the quantum Hamilton–Jacobi equation, a rate equation for the action function, is determined by the *quantum Lagrangian*, which is evaluated along the trajectory

$$\frac{dS}{dt} = \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - (V(x) + Q(x,t)) = L. \tag{1.7}$$

The quantum Lagrangian is the excess of the flow kinetic energy over the total potential energy, the latter now including the quantum potential in addition to the classical potential.

We are now in a position to summarize the three quantum trajectory equations of motion in Box 1.2. The equations of motion in the first half of this box are expressed in the Lagrangian frame, and the three subsidiary equations in the lower half relate the quantum potential and the density to the R-amplitude. In addition, the flow velocity is related to the gradient of the action.

Only two years after Bohm's papers appeared, Takabayasi presented a very different derivation of the hydrodynamic equations [3.1]. Rather than substituting the polar form of the wave function into the TDSE, he began with a quantum-mechanical distribution function, the Wigner function, in (x, p) phase space. This derivation will be presented in Chapter 3. (It was in 1932 that Wigner introduced a quantum phase space distribution function, $W(x, p, t)$, that has *some* features in common with the classical probability distribution [3.12].) Takabayasi's seminal contribution was to develop equations of motion for the *momentum moments* of the Wigner function. These moments are defined by the expression

$$\bar{p}_n(x,t) = \int_{-\infty}^{\infty} p^n W(x,p,t)dp. \tag{1.9}$$

The equations of motion for these moments form an infinite hierarchy, with the rate of change of one moment dependent on both lower and higher moments. For pure states, in which the state of the system is described by a wave function, the lowest two moments form a closed set, and the hierarchy terminates. Remarkably, the resulting equations for these moments are identical to the Bohm equations of motion for the probability density and the flow momentum.

The coupled rate equations for the momentum moments are applicable to both *pure states and statistical mixtures*. For *pure states*, when these equations are compared with the Lagrangian equations of motion in Box 1.2, it is revealed that the momentum appearing in the latter equations is the *average momentum* at each position x of the underlying phase space distribution function. Furthermore, for *mixed states*, a generalization of the quantum force has been derived [3.9–3.11] and this depends on the momentum spread of the phase space distribution function. During the course of developing these concepts are developed in Chapter 3, we will develop a deeper understanding of the trajectory equations, and the possibility of significant extensions to more general systems will be revealed (including dissipative systems coupled to a thermal environment). These studies will be described in Chapter 3, related methods for dissipative systems will be presented in Chapter 11, and in Chapter 12 we will use the momentum moments to develop trajectory representations for mixed quantum–classical systems.

1.3 The Quantum Trajectory Method

In the preceding section, we indicated that the equations of motion for quantum trajectories can be derived from two quite different viewpoints. In this section, it will be shown that these equations can be integrated *on the fly* to generate the density, action, and complex-valued wave function for an ensemble of quantum trajectories. In this *synthetic approach* to quantum hydrodynamics, the wave function is not precomputed in advance of the trajectory analysis; rather, the hydrodynamic fields and the quantum trajectories are computed concurrently. The *quantum trajectory method* (QTM), introduced by Lopreore and Wyatt in 1999 [4.1], is a computational implementation of the synthetic approach. The QTM will be described in this section, and many additional details will be presented in Chapter 4.

In the QTM, wave packet evolution is described in terms of a relatively small number of *correlated fluid elements* evolving along quantum trajectories. The QTM is initiated by discretizing the initial wave packet in terms of *N fluid elements*, small chunks of the probability amplitude. The equations of motion for the fluid elements are integrated in lockstep fashion, from one time step to the next. Along each quantum trajectory, the amplitude and action are computed by integrating two coupled equations of motion, and from these, the wave function is readily synthesized. These fluid elements are correlated with one another through the *quantum potential*, from which is derived the quantum force. *Through the quantum potential, each fluid element is influenced by the motions of the other elements, and the ensuing correlation brings all quantum effects into the dynamics.*